

chain nodes :

7 8 9 10 11 12 13 15 16 23 24 25 26 27 28

ring nodes :

1 2 3 4 5 6

chain bonds :

2-23 5-7 7-8 7-15 7-16 8-9 8-10 10-11 11-12 12-13 23-24 24-25  
24-28 25-26 26-27

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-2 1-6 2-3 2-23 3-4 4-5 5-6 5-7 7-15 7-16 8-9 10-11 11-12  
12-13 24-25 24-28 25-26 26-27

exact bonds :

7-8 8-10 23-24

isolated ring systems :

containing 1 :

G1:O,S,N

G2:H,CH3

G3:O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 11:CLASS 12:CLASS 13:Atom 15:CLASS 16:CLASS 23:CLASS  
24:CLASS 25:CLASS 26:CLASS 27:Atom 28:CLASS

Generic attributes :

13:  
Saturation : Unsaturated  
27:  
Saturation : Unsaturated

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Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading structure

L7 STRUCTURE UPLOADED

=> s 17

SAMPLE SEARCH INITIATED 11:33:53 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 243 TO ITERATE

100.0% PROCESSED 243 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 3925 TO 5795  
 PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s 17 sss full

FULL SEARCH INITIATED 11:35:38 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 5026 TO ITERATE

100.0% PROCESSED 5026 ITERATIONS 12 ANSWERS  
 SEARCH TIME: 00.00.01

L9 12 SEA SSS FUL L7

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	167.35	346.20
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.73

FILE 'CAPLUS' ENTERED AT 11:35:45 ON 02 OCT 2005  
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FILE COVERS 1907 - 2 Oct 2005 VOL 143 ISS 15

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FILE LAST UPDATED: 30 Sep 2005 (20050930/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=&gt; s 19

L10 3 L9

=&gt; d l10 1-3 bib abs hitstr

L10 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

Full Text

AN 2004:515509 CAPLUS

DN 141:71566

TI Preparation of hydroxybenzothiazolyloxypropylpiperazines as fatty acid oxidation inhibitors.

IN Elzein, Elfatih; Koltun, Dmitry; Zablocki, Jeff

PA CV Therapeutics, Inc., USA

SO PCT Int. Appl., 68 pp.

CODEN: PIXXD2

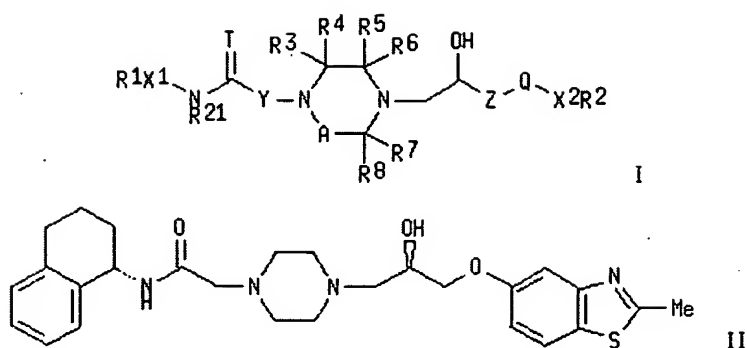
DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004052887	A2	20040624	WO 2003-US38867	20031205
	WO 2004052887	A3	20040715		
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	RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
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	US 2004152890	A1	20040805	US 2003-729499	20031205
	EP 1567525	A2	20050831	EP 2003-812835	20031205
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
PRAI	US 2002-431506P	P	20021205		
	WO 2003-US38867	W	20031205		
OS	MARPAT 141:71566				
GI					

Apps



AB Title compds. [I; R1, R2 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, heteroaryl; X1 = bond, (CR15R16)p; X2 = bond, (CR18R19)q; R15, R16 = H, OH, alkyl, CO2R17; R17 = H, alkyl, (substituted) Ph; n, p, q = 1-3; R21 = H, alkyl; T = O, S; Y, Z = (CR18R19)q; R11, R12, R13, R14, R18, R19 = H, alkyl; A = (CR9R10)m; m = 1, 2; R3-R10 = H, alkyl, COR; R = OR11, NR11R12; R3R4, R5R6, R7R8, R9R10 = O; R3R7, R3R9, R5R7, R5R9 = (CR13R14)n; Q = O, S, NR20; R20 = H, (substituted) alkyl; with provisos], were claimed. Title compd. (II) inhibited palmitoyl CoA oxidn. with IC50 = 0.08  $\mu$ M.

IT 678982-07-5P 678982-12-2P 709041-43-0P

709041-44-1P 709041-45-2P

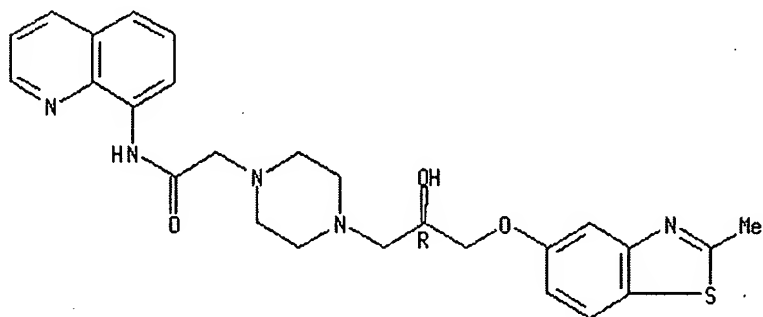
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compd.; prepn. of hydroxybenzothiazolyloxypropylpiperazines as fatty acid oxidn. inhibitors)

RN 678982-07-5 CAPLUS

CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-N-8-quinolinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

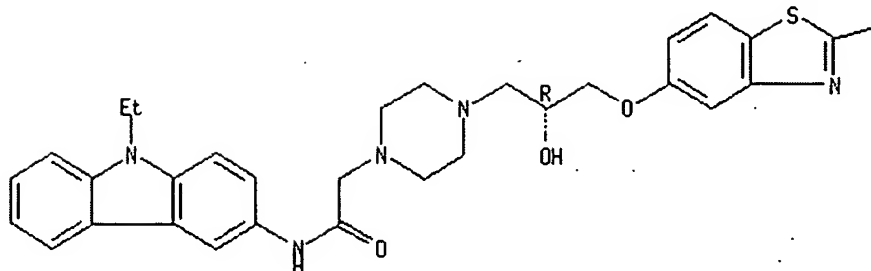


RN 678982-12-2 CAPLUS

CN 1-Piperazineacetamide, N-(9-ethyl-9H-carbazol-3-yl)-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

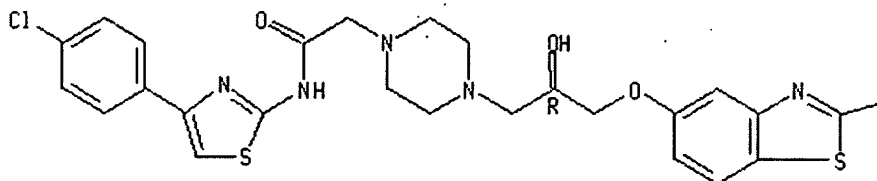
— Me

RN 709041-43-0 CAPLUS

CN 1-Piperazineacetamide, N-[4-(4-chlorophenyl)-2-thiazolyl]-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

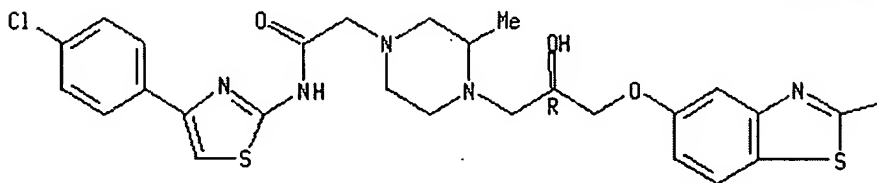
— Me

RN 709041-44-1 CAPLUS

CN 1-Piperazineacetamide, N-[4-(4-chlorophenyl)-2-thiazolyl]-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

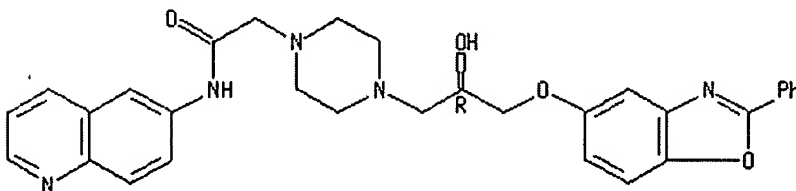
PAGE 1-A



—Me

RN 709041-45-2 CAPLUS  
 CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-[(2-phenyl-5-benzoxazolyl)oxy]propyl]-N-6-quinolinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



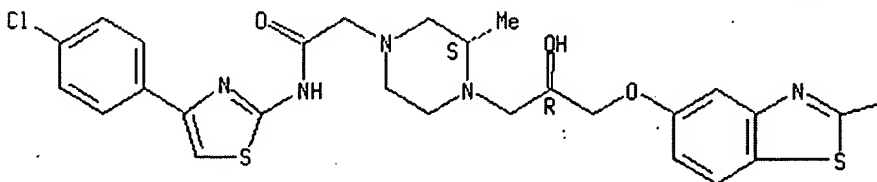
IT 709041-49-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of hydroxybenzothiazolyloxypropylpiperazines as fatty acid oxidn. inhibitors)

RN 709041-49-6 CAPLUS  
 CN 1-Piperazineacetamide, N-[4-(4-chlorophenyl)-2-thiazolyl]-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-3-methyl-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



PAGE 1-A

PAGE 1-B

—Me

L10 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

Full Text

AN 2003:1002009 CAPLUS

DN 140:331785

TI New fatty acid oxidation inhibitors with increased potency lacking adverse metabolic and electrophysiological properties

AU Koltun, Dmitry O.; Marquart, Timothy A.; Shenk, Kevin D.; Elzein, Elfatih;

Li, Yuan; Nguyen, Marie; Kerwar, Suresh; Zeng, Dewan; Chu, Nancy; Soohoo, Daniel; Hao, Jia; Maydanik, Victoria Y.; Lustig, David A.; Ng, Khing-Jow; Fraser, Heather; Zablocki, Jeffery A.

CS Department of Bioorganic Chemistry, Palo Alto, CA, 94304, USA

SO Bioorganic Medicinal Chemistry Letters (2004), 14(2), 549-552

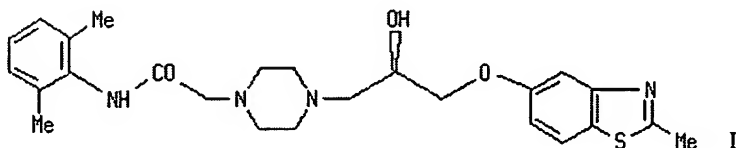
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

LA English

GI



AB New inhibitors of palmitoylCoA oxidn. were synthesized based on a structurally novel lead, CVT-3501 (I). Investigation of structure-activity relationships was conducted with respect to potency of inhibition of cardiac mitochondrial palmitoylCoA oxidn. and metabolic stability. Three potent and metabolically stable analogs were evaluated in vitro for cytochrome P 450 inhibition and potentially adverse electrophysiol. effects. One compd. (II) was also found to have favorable pharmacokinetic properties in rat.

IT 678982-12-2P

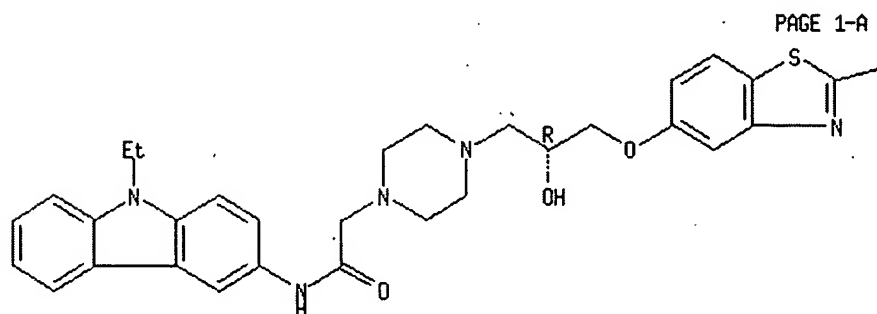
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(fatty acid oxidn. inhibitors with increased potency lacking adverse metabolic and electrophysiol. properties)

RN 678982-12-2 CAPLUS

CN 1-Piperazineacetamide, N-(9-ethyl-9H-carbazol-3-yl)-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



PAGE 1-B

Me

IT 678982-06-4P 678982-07-5P 678982-08-6P



# STN Columbus

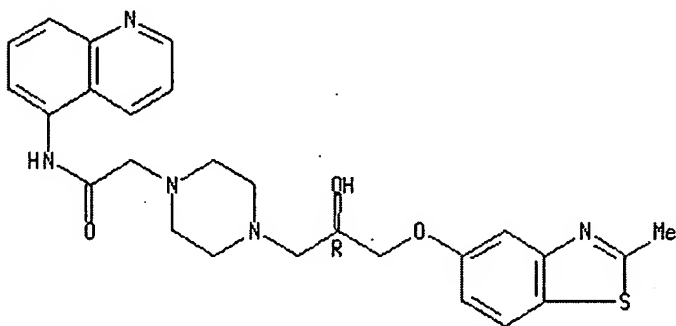
678982-09-7P 678982-10-0P 678982-11-1P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(fatty acid oxidn. inhibitors with increased potency lacking adverse metabolic and electrophysiol. properties)

RN 678982-06-4 CAPLUS

CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-N-5-quinolinyl- (9CI) (CA INDEX NAME)

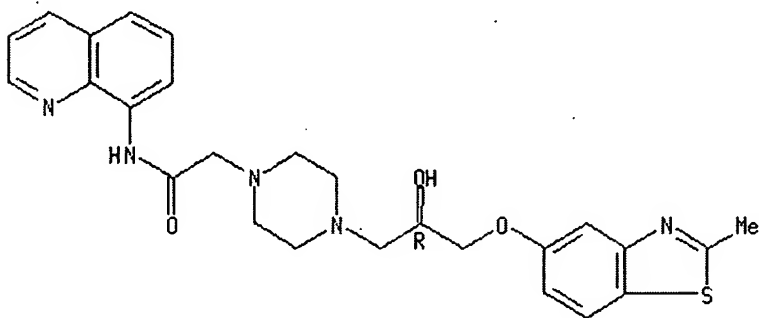
Absolute stereochemistry.



RN 678982-07-5 CAPLUS

CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-N-8-quinolinyl- (9CI) (CA INDEX NAME)

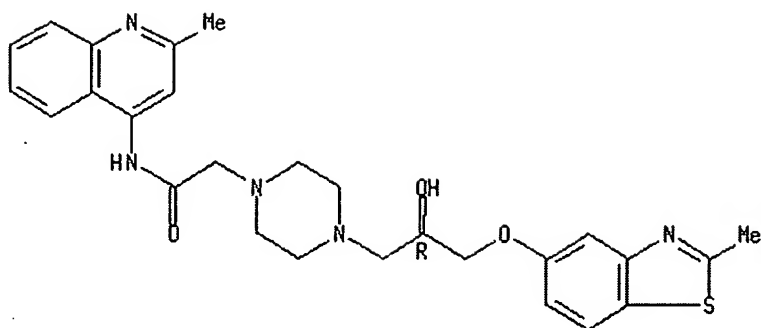
Absolute stereochemistry.



RN 678982-08-6 CAPLUS

CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-N-(2-methyl-4-quinolinyl)- (9CI) (CA INDEX NAME)

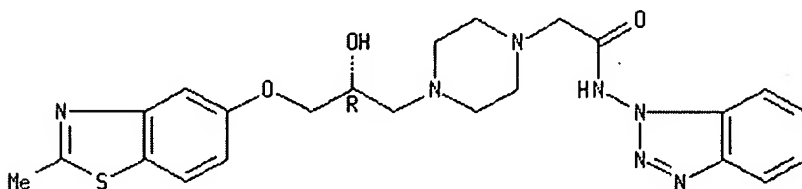
Absolute stereochemistry.



RN 678982-09-7 CAPLUS

CN 1-Piperazineacetamide, N-1H-benzotriazol-1-yl-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]- (9CI) (CA INDEX NAME)

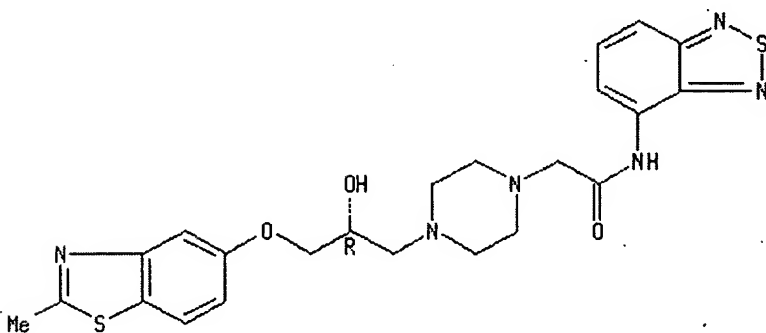
Absolute stereochemistry.



RN 678982-10-0 CAPLUS

CN 1-Piperazineacetamide, N-2,1,3-benzothiadiazol-4-yl-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]- (9CI) (CA INDEX NAME)

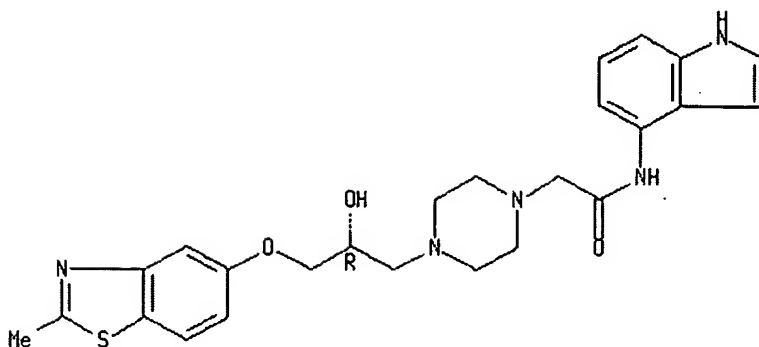
Absolute stereochemistry.



RN 678982-11-1 CAPLUS

CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-N-1H-indol-4-yl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

Full Text

AN 2002:314915 CAPLUS

DN 136:340700

TI Preparation of 4-[3-heteroaryloxy-2-hydroxypropyl]-1-piperazineacetamides  
as P-glycoprotein and/or MRP1 inhibitors for treating multidrug resistance

IN Degenhardt, Charles Raymond; Eickhoff, David Joseph

PA The Procter Gamble Company, USA

SO PCT Int. Appl., 66 pp.

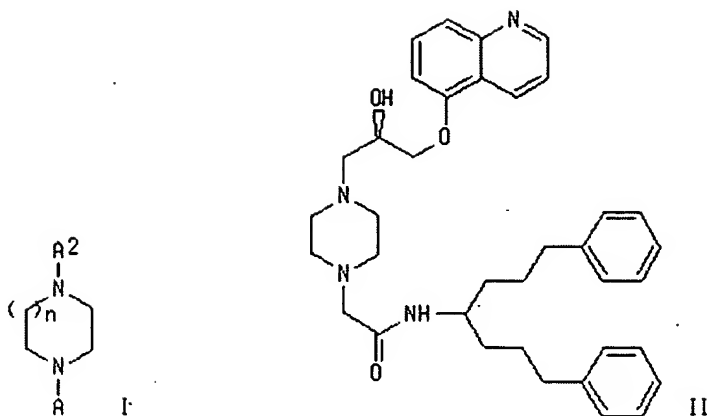
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 4

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PI	WO 2002032874	A2	20020425	WO 2001-US32422	20011016
	WO 2002032874	C1	20031113		
	WO 2002032874	A3	20020725		
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	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
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	US 6693099	B2	20040217		
	CA 2420996	AA	20020425	CA 2001-2420996	20011016
	AU 2002013336	A5	20020429	AU 2002-13336	20011016
	EP 1326840	A2	20030716	EP 2001-981711	20011016
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	US 2004132722	A1	20040708	US 2003-741270	20031219
PRAI	US 2000-241127P	P	20001017		
	US 2000-740391	A	20001219		
	WO 2001-US32422	W	20011016		
OS	MARPAT 136:340700				
GI					



AB Title compds. I [wherein n = 1-3; A = A<sub>1</sub> or A<sub>3</sub>; A<sub>1</sub> = (CR<sub>1</sub>R<sub>1</sub>)xD<sub>1</sub>OyD<sub>2</sub>zR<sub>2</sub>; R<sub>1</sub> = independently H, OH, (un)substituted hydrocarbon, heterogeneous group, carboxylic group, heterocyclic, or (hetero)arom.; x = 0-10; R<sub>2</sub> = (un)substituted hydrocarbon, heterogeneous group, carboxylic group, heterocyclic, or (hetero)arom.; D<sub>1</sub> and D<sub>2</sub> = independently CO or NR<sub>3</sub>; R<sub>3</sub> = H or R<sub>2</sub>; or R<sub>2</sub>R<sub>3</sub> may form a heterocycle; y = 0-1 and z = 0-1 with provisos; A<sub>2</sub> = (CR<sub>1</sub>R<sub>1</sub>)uD<sub>3</sub>(CR<sub>1</sub>R<sub>1</sub>)pOvR<sub>5</sub>; u = 0-10; p = 0-10; v = 0-1; D<sub>3</sub> = SO<sub>2</sub>, CO, or CR<sub>1</sub>OH with provisos; R<sub>5</sub> = substituted hydrocarbon or heterogeneous group; A<sub>3</sub> = D<sub>4</sub>(CR<sub>1</sub>R<sub>1</sub>)tD<sub>5</sub>; t = 1-6; D<sub>4</sub> = CO or CHR<sub>1</sub>; D<sub>5</sub> = NR<sub>6</sub>R<sub>7</sub>, OrR<sub>6</sub>, or COR<sub>6</sub>; r = 0-1; R<sub>6</sub> = (un)substituted hydrocarbon, heterogeneous group, carboxylic group, heterocyclic, or (hetero)arom.; R<sub>7</sub> = H or R<sub>6</sub> with provisos; or optical isomers, diastereomers, enantiomers, pharmaceutically acceptable salts, or biohydrolyzable amides, esters, or imides thereof] were prep'd. as P-glycoprotein and/or MRP1 inhibitors for treating multidrug resistance. For example, lithium 4-(tert-butoxycarbonyl)-1-(carboxymethyl)piperazine (prepn. given) was amidated with 1,7-diphenyl-4-heptylamine•HCl in the presence of 1-hydroxybenzotriazole, N,N-diisopropylethylamine, and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide in DMF. Deprotection and addn. of (R)-5-oxiranylmethoxyquinoline afforded II. The latter exhibited an accumulation index (ratio of fluorescence in the presence of modulator to fluorescence in the absence of modulator) of 10 in NIH-MDR1-G185 cells. I are useful as cancer therapeutic agents, antibacterial agents, antiviral agents, and antifungal agents (no data). Compns. of the substituted heterocyclic compds. are also disclosed.

IT 416857-33-5P, N-[1-[2-(R)-Hydroxy-3-(quinolin-5-yloxy)propyl]piperazine-4-acetyl]-3-(3-pyridyl)alanine [4-phenyl-1-(3-phenylpropyl)butyl]amide

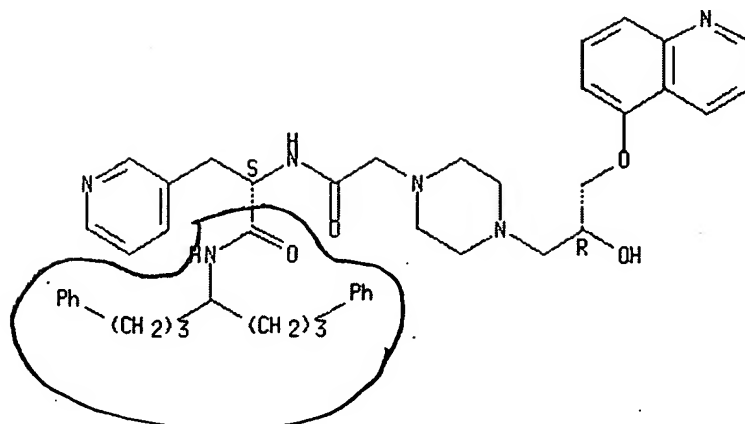
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Pgp and/or MRP1 inhibitor; prep'n. of heteroaryloxyhydroxypropyl piperazineacetamides as P-glycoprotein or MRP1 inhibitors for treating multidrug resistance)

RN 416857-33-5 CAPLUS

CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-(5-quinolinylloxy)propyl]-N-[(1S)-2-oxo-2-[[4-phenyl-1-(3-phenylpropyl)butyl]amino]-1-(3-pyridinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=&gt; file caold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

15.27

361.47

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-2.19

-2.92

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=&gt; d his

(FILE 'HOME' ENTERED AT 11:11:58 ON 02 OCT 2005)

FILE 'REGISTRY' ENTERED AT 11:12:20 ON 02 OCT 2005

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 31 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:20:28 ON 02 OCT 2005

L4 1 S L3

FILE 'CAOLD' ENTERED AT 11:20:59 ON 02 OCT 2005

L5 0 S L3

FILE 'REGISTRY' ENTERED AT 11:25:37 ON 02 OCT 2005

# STN Columbus

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L6 65 S VASOPRESSIN AND REVIEW AND CURRENT

FILE 'REGISTRY' ENTERED AT 11:27:00 ON 02 OCT 2005  
L7 STRUCTURE UPLOADED  
L8 0 S L7  
L9 12 S L7 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:35:45 ON 02 OCT 2005  
L10 3 S L9

FILE 'CAOLD' ENTERED AT 11:36:25 ON 02 OCT 2005

=> s 19  
L11 0 L9

=>